4 de DICIEMBRE de 2024

12.00 h Sala de Grados, Ed. A Facultad de Ciencias, Campus San Francisco

INMA Junior

"Multifunctional derivatives of zwitterionic 2-pyridones and their potential application"

Aleksandra Mašulović CLIP Group, INMA-CSIC/UNIZAR

Azo dyes exhibit diverse topologies and intriguing structures, directly influenced by their building blocks, leading to notable properties. When *N*-substituted pyridone is used, disperse dyes display vivid colors, excellent lightfastness, and high extinction coefficients. Pyridine-based dyes improve dyeing properties, sublimation, and brightness on various fibers. However, challenges like alkali-unstable hydroxyl groups and water insolubility limit their application, traditionally requiring acidic conditions for stability. Thus, a high motivation for new molecular design and study of innovative dyes which will satisfy the mentioned requirements arises. Herein, two series of azo dyes based on 6-hydroxy-4-methyl-3-pyridinium-2-pyridone were obtained in the form of zwitterions. The application potential of 2-pyridone derivatives was examined by determination of their antioxidant, antimicrobial and anticancer activities. Moreover, their tautomeric features were discussed. It was observed that the dyes protonated form is cationic, while their deprotonated form is zwitterionic. The application potential was examined by determination of biological activities as well as by dying fabrics of different chemical composition: diacetate, bleached cotton, naylon, polyester, polyacriloniterile, wool. Considering the preformed characterization, it was shown that the dye-fabric adhesion depends on the dye form wherein the zwitterionic form interacts with fabric faster, while the hydrazone form establishes firmer interactions. The dye-fabric interactions were elucidated depending on the molecular structure of the dyes, with regard to the electronic effects of the substituents.

"Synthesis and properties of novel azo dyes and compounds based on pyridinium iodide for the application in dye-sensitized solar cells"

Luka Matović CLIP Group, INMA-CSIC/UNIZAR

Dye-sensitized solar cells (DSSCs) represent a cleaner and more sustainable energy solution than conventional fossil fuels, effectively addressing major environmental, economic, and practical issues associated with traditional energy systems. While there are ongoing challenges, such as improving long-term stability and efficiency, the inherent advantages of DSSCs position them as a valuable technology for expanding renewable energy adoption and enabling innovative energy applications. This work encompassed the synthesis, characterization, and determination of physico-chemical, photophysical, and electronic properties of two series of compounds for potential application in assembled DSSCs. The first series comprised six azo compounds which were utilized as photosensitizers, while the second series included five compounds based on pyridinium iodide employed as additional redox components to the commercial iodine-based liquid electrolyte (LiI+1₂). The key photovoltaic parameters of all assembled DSSCs were determined and compared to those of a reference DSSC comprising commercial N719 dye as the photosensitizer, titanium(IV) oxide (TiO₂) as the semiconductor, and a commercial iodine-based liquid electrolyte. The DSSCs employing azo dyes as photosensitizers exhibited competitive conversion efficiencies compared to the DSSC utilizing the commercial N719 dye. Furthermore, the DSSCs incorporating compounds based on pyridinium iodide as supplementary electrolyte components achieved enhanced photovoltaic performance compared to the DSSC utilizing a commercial iodine-based liquid electrolyte without additives.







